Geophysical Research Abstracts
Vol. 13, EGU2011-716, 2011
EGU General Assembly 2011
© Author(s) 2010

Modeling the dissolution of calcite coupled to gypsum precipitation in acid brines

Maria Gabriela Davila Ordoñez, Maria Garcia Rios, Josep M. Soler, and Jordi Cama
Spain (gaba1983@hotmail.com)

Gabriela Dávila1, Maria García-Rios1,2, Josep M. Soler1 and Jordi Cama1
1Departament de Geociències, Institut de Diagnosi Ambiental i Estudis de l'Aigua (IDAEA, CSIC). Jordi Girona 18-26, Barcelona 08034, Catalonia, Spain
2Fundación Ciudad de la Energía (CIUDEN). Avenida de Compostilla 2, Ponferrada 24400, Spain

The injection of CO2 into repository rocks made up of limestones and dolostones (e.g., the test site in Hontomín, Spain) will cause the formation of CO2-rich acid brines, which will induce the dissolution of the carbonate minerals (calcite and dolomite). Since the brine contains sulfate, gypsum (or anhydrite at depth) will precipitate, which may coat the surface of the dissolving carbonate, causing its passivation. These reactions imply changes in porosity and in the structure of pores in the repository rock. Therefore, changes in permeability and fluid flow are expected.

Flow-through experiments are carried out to study the kinetics of the dissolution of calcite coupled to the precipitation of gypsum at atmospheric PCO2. An acidic solution at equilibrium with gypsum is continually injected into a cell containing a known mass of calcite grains.

The experimental results are simulated using the reactive transport code TRACONF-CHEPROO. The experimental conditions such as the amount of mass, surface area, cell volume, flow rate, temperature, pressure, etc, are considered in the modeling. The kinetic parameters used are obtained from the literature. Thus, comparison between experimental and simulated results is crucial to obtain the proper kinetic parameters.

An acidic solution (H2SO4, pH 2.5) at equilibrium with gypsum is continually injected to react with a known mass of calcite, with a grain size between 1 and 2 mm. Knowing the dissolution rate law for calcite, its surface area (0.5 m2/g, measured by BET), the volume of solution in the cell and the flow rate, the expected evolution of the solution composition at the outlet of the reaction cell is calculated. Simulations of the experimental results overestimate the dissolution rate of calcite (large increase in pH and Ca concentration). A rapid decrease in sulfate concentration is caused by the precipitation of gypsum, and the model predicts the complete dissolution of calcite.

To refine the model the reactive surface area of calcite was decreased until a match between model and experimental results is achieved. The reason for this apparently small reactive surface area probably resides in the effect caused by gypsum precipitating directly on the surfaces of the calcite grains, causing a passivation of the reacting calcite.